Hierarchical alternating nonlinear least squares for nonnegative matrix factorization using rational functions

Cécile Hautecoeur, François Glineur and Lieven De Lathauwer

UCLouvain, CORE & ICTEAM/INMA institutes - KU Leuven, ESAT-STADIUS

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Contribution of this work

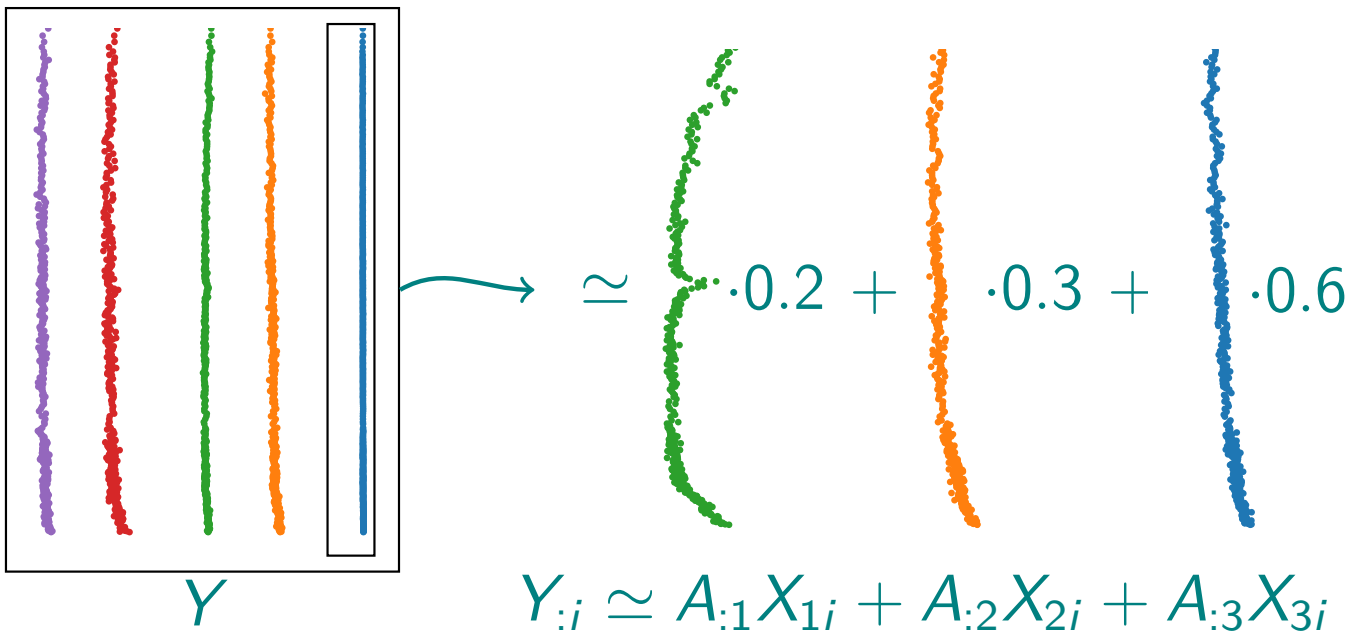
- **Previous work:**
  - Nonnegative Matrix Factorization (NMF) = **linear dimension reduction technique**, doing nonnegative decompositions
  - NMF using **polynomials or splines** = **smoother and more accurate** decomposition
- **Contributions**
  - NMF using **rational functions** = **better** than polynomials and splines **for denoising and reconstruction** of some synthetic and real-world datasets.

Nonnegative Matrix Factorization (NMF)

Widely used linear dimension reduction technique for nonnegative data

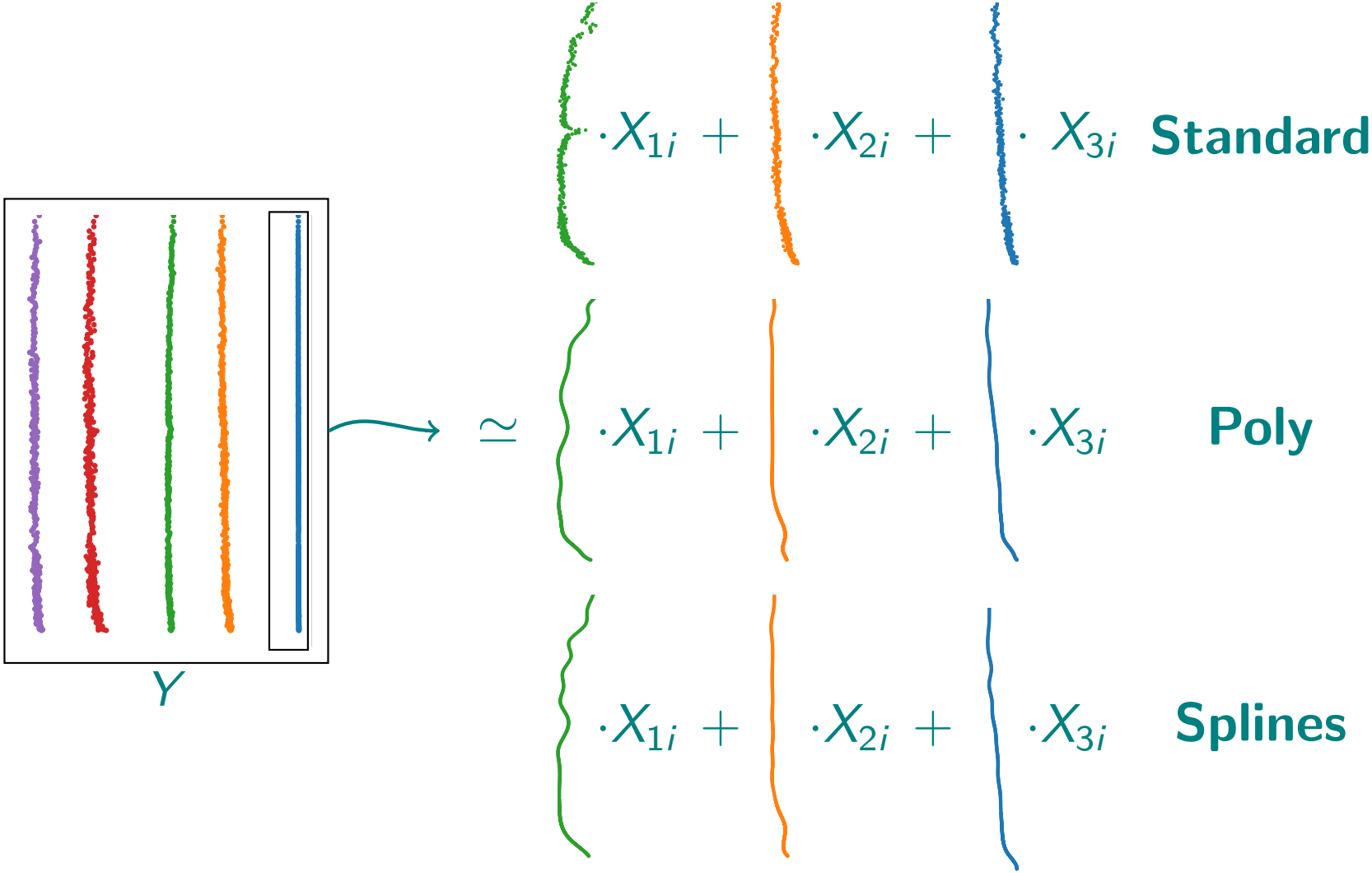
Given an input matrix $Y \in \mathbb{R}^{m \times n}$ and a factorization rank r, find **nonnegative** matrices $A \in \mathbb{R}_+^{m \times r}$, and $X \in \mathbb{R}_+^{r \times n}$ solving $Y \simeq AX$:

$$\min_{A \in \mathbb{R}_+^{m \times r}, X \in \mathbb{R}_+^{r \times n}} ||Y - AX||_F^2 = \sum_{i=1}^{n} \left|\left| Y_{:i} - \sum_{j=1}^{r} A_{:j} X_{ji} \right|\right|^2.$$



NMF on polynomials or splines

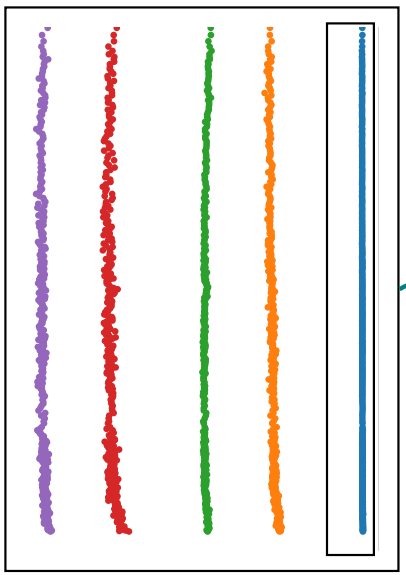
A way of smoothing the signals in A



[Zdunek & al., 2014, Debals & al. 2018, Hautecoeur & Glineur 2020]

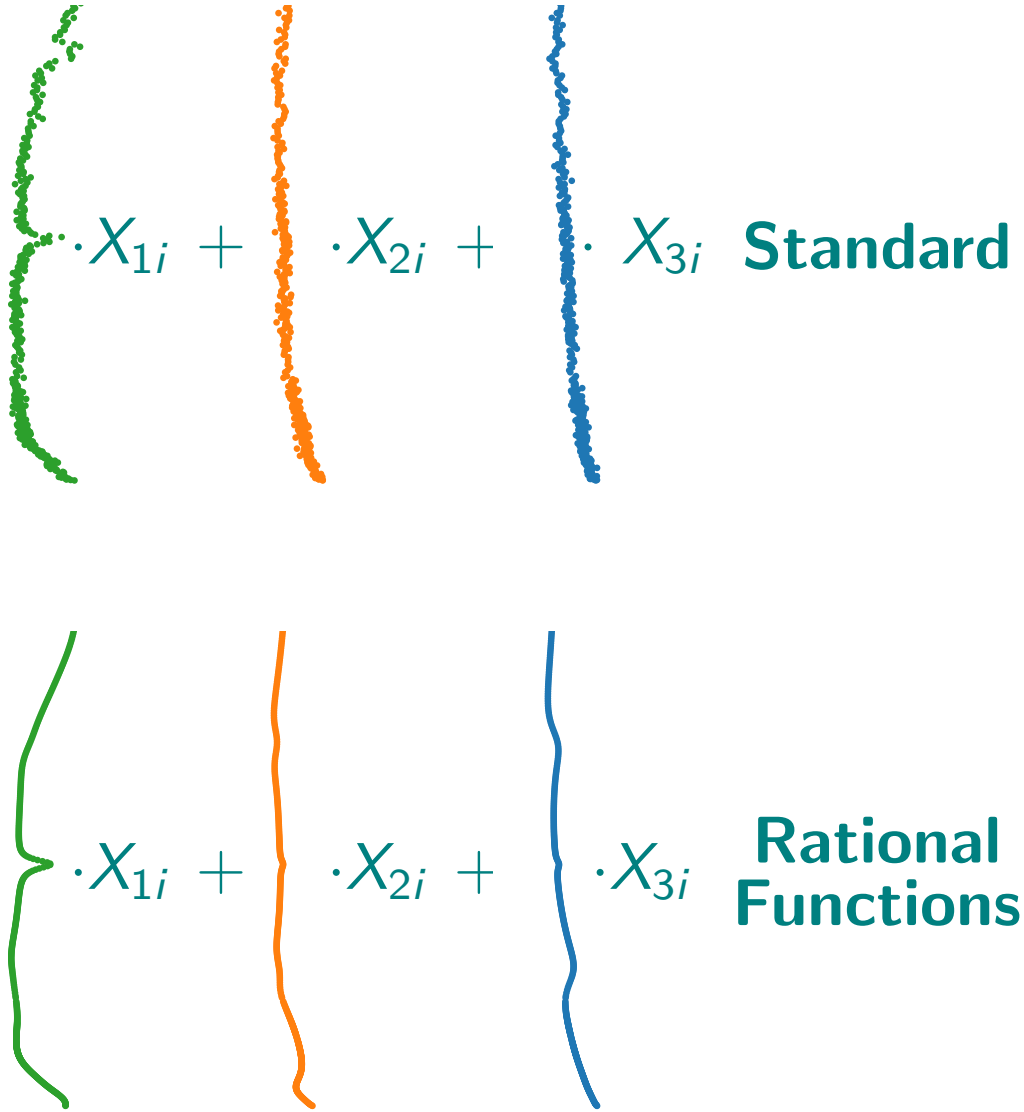
NMF on rational functions

To be able to represent spikes in A

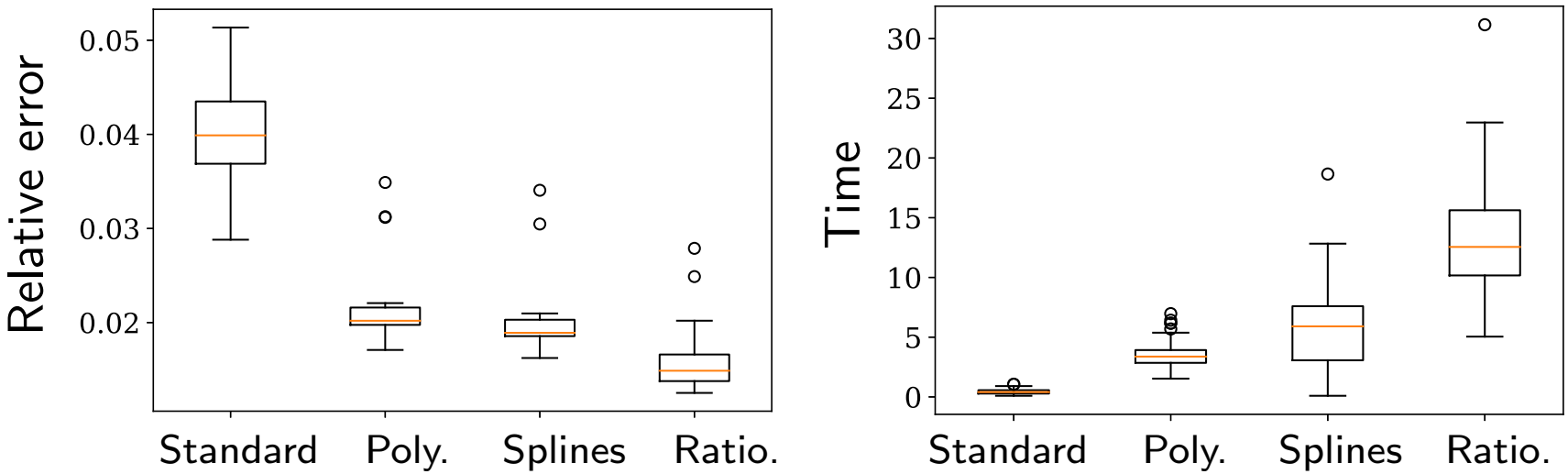


Y

$\rightarrow \simeq$



Performances on synthetic data:

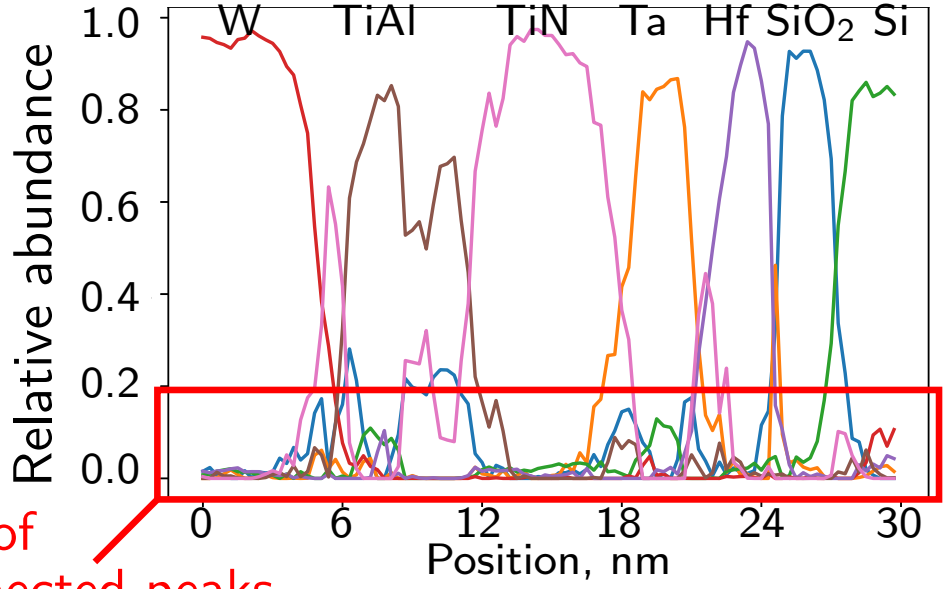


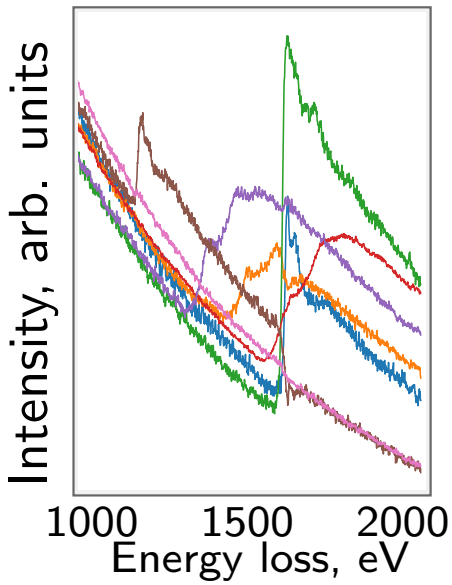
Boxplots of the relative error (left) and the computation time (right), for different models solving NMF problem

The use of rational functions significantly **outperforms existing methods** in terms of **denoising and reconstruction ability**, at the cost of an increase in computational time.

Unmixing spectrum images of multicomponent nanostructures

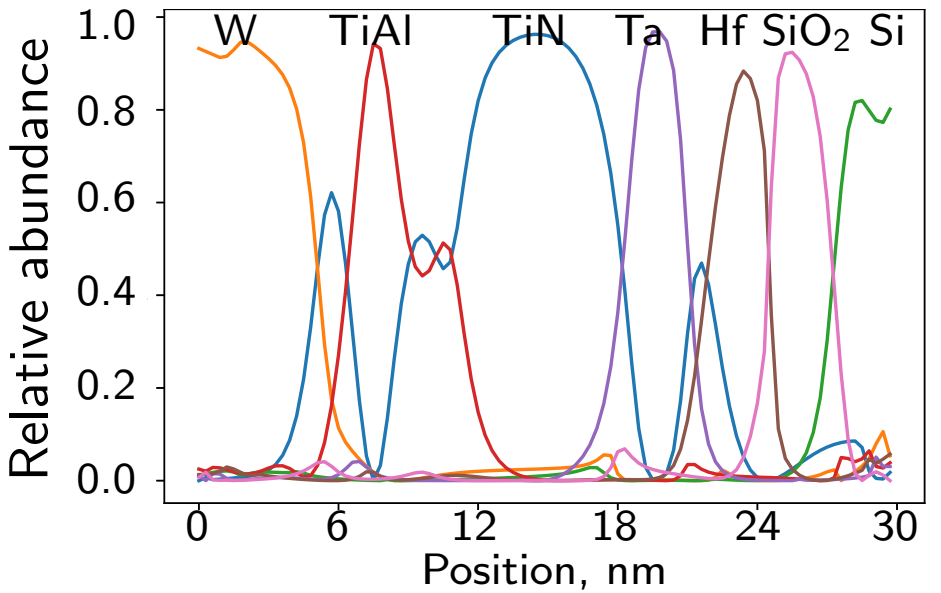
Standard

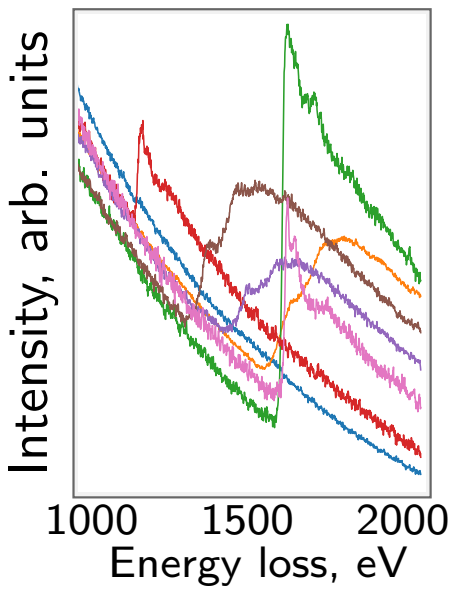




Lots of unexpected peaks

Rational Functions





→ Using rational functions leads to **smoother** and **more realistic** results